

# **Biology and Environmental Science Working Group**

## **Summary Viewgraphs**

# **Study of Atmospheric Aerosols by Laser Post Ionization Time-of-Flight Mass Spectrometry at the Argonne Free Electron Laser Facility**

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Argonne National Laboratory**



# LPI TOF MS

- ⇒ single particle analysis
- ⇒ chemical speciation possible
- ⇒ quantification possible
- ⇒ depth profiling – **bulk and surface** analysis possible

# Projected Outcome of SPI ToF MS on Aerosols

- information about single particle composition
  - ⇒ surface and bulk composition, provides insight whether **internally** or **externally** mixed
  - ⇒ surface **coating**?
  - ⇒ reaction potential of the particle
- together with bulk chemical composition, **radiative properties** can be estimated

# **Analysis of Biological Samples (with no matrix) Using Large Gold Cluster Bombardment and an orthogonal TOFMS**

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# ***OUR APPROACH FOR ANALYSIS OF PEPTIDES***

- 10-20 keV  $\text{Au}_n^+$  ( $n = 1-3-5-9$ ) and  **$\text{Au}_{400}^{4+}$**  clusters as **Primary Ions**
- **Orthogonal Extraction** Time of Flight Mass Spectrometer

# CONCLUSIONS

- Enhanced Secondary Ion Yield

	$\text{Au}^+$	$\text{Au}_3^+$	$\text{Au}_5^+$	$\text{Au}_9^+$	$\text{Au}_{400}^{4+}$
yield enhancement	1	50	100	310	900

- Significantly Improved Signal-to-noise Ratio
- Reduced Fragmentation
- Very Low Surface Damage

$\text{Au}_{400}^{4+}$  may enhance SIMS sensitivity of large biomolecules PROTEINS/OLIGONUCLEOTIDES??

# Analyzing Nanoscale Organic Surfaces – From Conducting Polymers to Biomaterials

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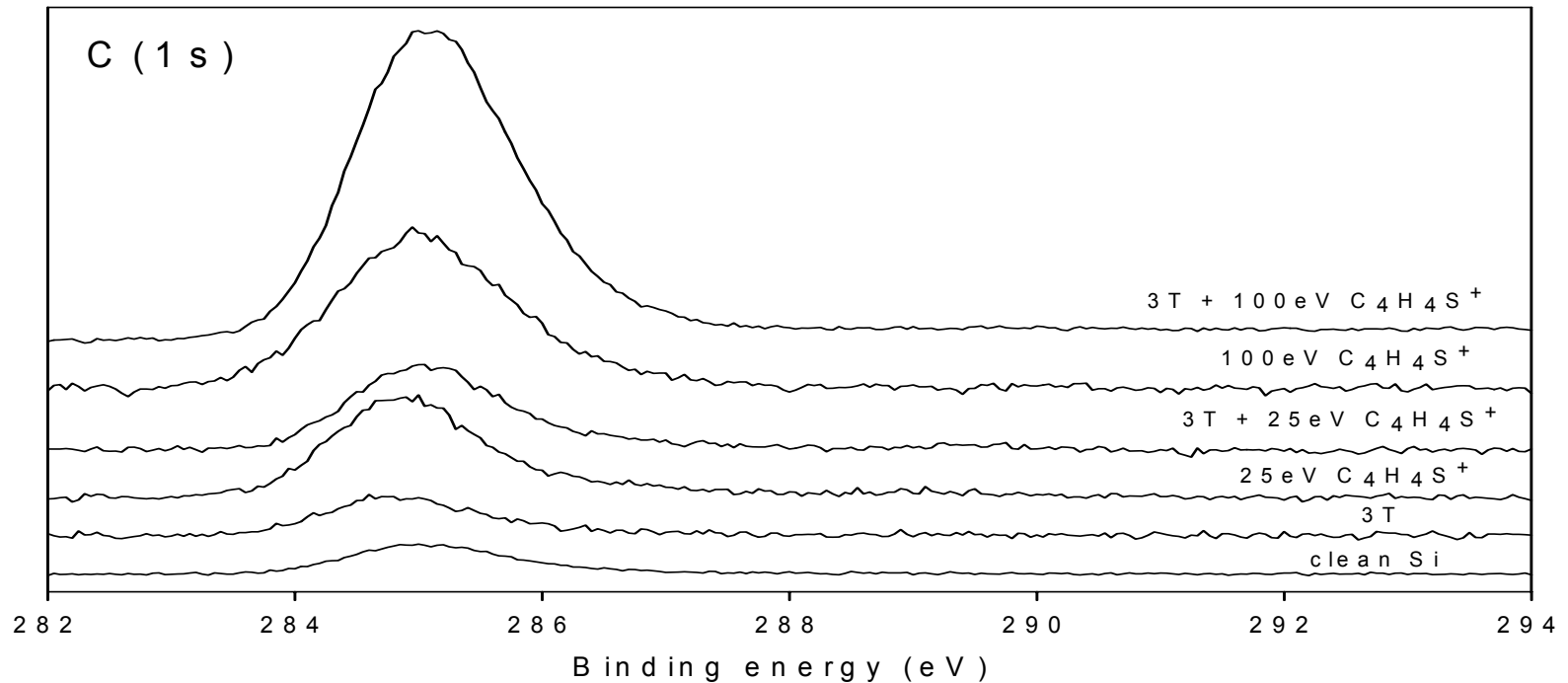
# **Problems with Organic Film Analysis by X-ray Photoelectron Spectroscopy**

Cannot see entire chemical structure

- Molecular weight
- Relation of diff. functional groups

All organic films do not have well resolved peaks in x-ray photoelectron spectroscopy

# X-ray Photoelectron Spectroscopy: C(1s) of Various Polythiophene Conducting Polymer Films

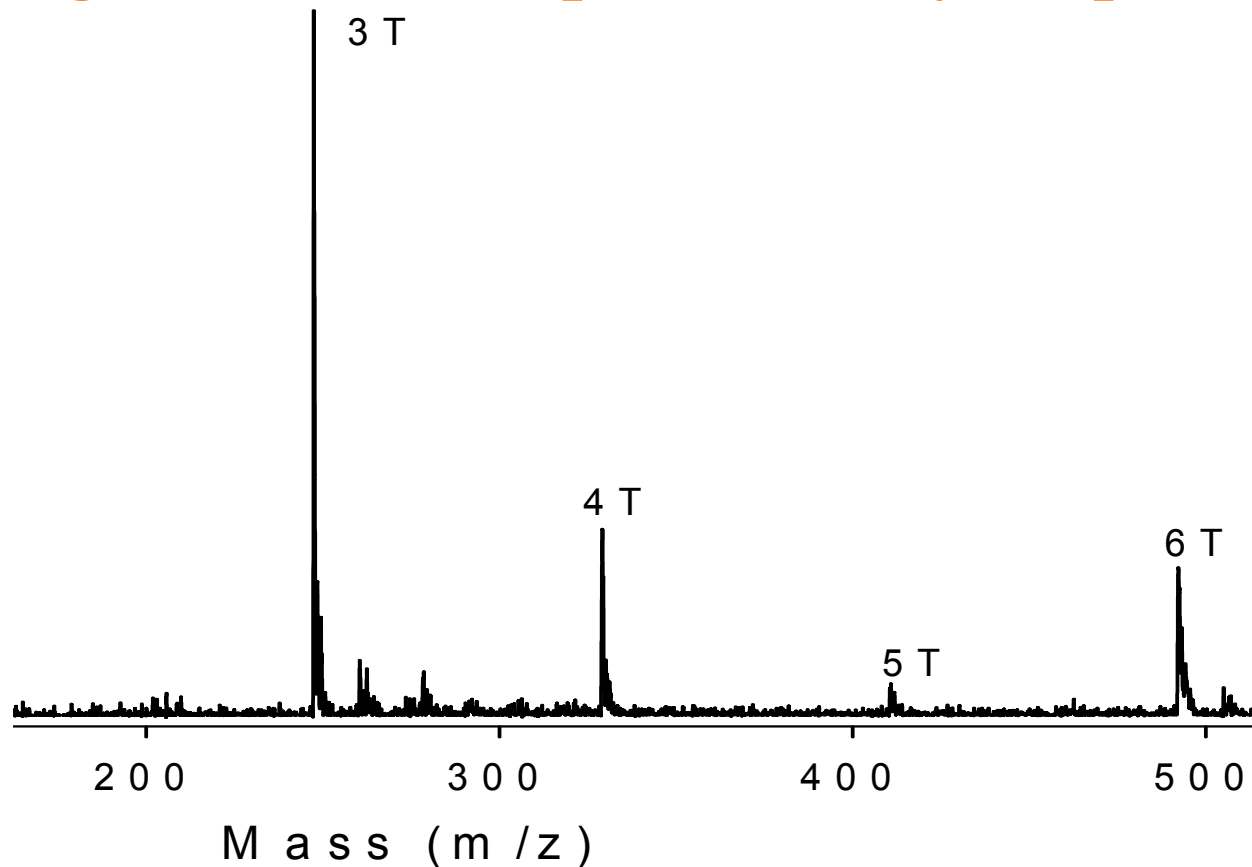


## Analysis Problem in XPS:

**Insufficient chemical resolution →**

**Films show similar C(1s) but different optical activity**

# Single Laser Desorption of Polythiophene



- Polymerization: Form distribution of species: 3T, 4T, 5T, 6T
- Are these fragments or intact species?
- FEL for SPI of laser/ion desorbed neutrals

# **Electronic Structure of Conducting Polymers:**

## **Fluorescence of Polythiophene Films**

Related Biological/Environmental Problems:

Charge transfer at organic/inorganic interfaces

- Solar cells
- Photocatalytic degradation of pollutants
- Tissue electrostimulation (Pacemaker,...)

# SPI for Mixtures, Large Molecules & Surfaces

- Problems of poor ionization & complex mass spectra
- Utilize multiple desorption/volatization methods
- Various applications
  - Protein MS, sugars, non-covalent complexes,...
  - Organic, polymer, biological film/surface analysis
- Overarching issues with SPI of molecules
  - Optimal wavelength unknown → Tune 7 – 20 eV
  - High power needed to saturate process
  - How much fragmentation occurs? Neutral's internal energy
  - What is mass limit of ionization? Stability of cations?
- Instrumental Issues
  - Proposed FEL parameters nearly ideal for SPI
  - FEL to prove concept for lab source development
  - Synchronize FEL to pulsed desorption methods
  - Beyond FEL: Much can be done with SPIRIT

## **Using ALFF for Two Photon Photoemission Spectroscopy (2PPE)**

- Shorter wavelengths:  $\lambda < 205$  nm
- 2 color experiment
  - UV/Vis fs laser for pump
  - ALFF for probe
- Vacuum system compatible with organics
  - Usually UHV, single substrate expt
  - Contamination by organic sample outgassing